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NUMERICAL HYDRODYNAMIC CALCULATIONS OF THE FLOW OF THE
DETONATION PRODUCTS FROM A POINT-INITIATED EXPLOSIVE CYLINDER

By

D. Piacesi, Jr.

ABSTRACT: With the use of the NOL two-dimensional hydrodynamics computer program (CYCLONE), a detailed numerical analysis is made of the flow in the product-gas of a detonating cylinder of pentolite (50/50 PETN/TNT) explosive. The explosive cylinder is initiated at a point on the central charge axis at one end-face. The detonation front is assumed to be spherical. This is consistent with experimentally determined wave shapes. The calculations are carried out to the point where the detonation front is at 1.71-charge-diameters from the point of initiation. The results of the calculations show that the flow in the "detonation head" (region bounded by the detonation front, and the lateral and rear rarefaction waves) is entirely spherical. Moreover, this spherical flow is exactly that which is described by the similarity solution of G. I. Taylor for a spherical detonation wave.

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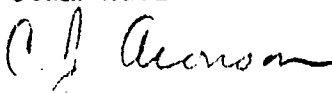
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NUMERICAL HYDRODYNAMIC CALCULATIONS OF THE FLOW OF THE
DETONATION PRODUCTS FROM A POINT-INITIATED EXPLOSIVE CYLINDER

This report discusses the results of numerical hydrodynamic calculations on the flow in the product-gas resulting from the detonation of a cylinder of explosive. This report will be of interest to scientists who are dealing with experiments involving point-initiated explosive cylinders, and to engineers concerned with conventional explosive weapons design. This work was carried out under NAVORD Task ORD-033-221/092-1/F008-08-11 Problem 004 - Explosion Hydrodynamic Calculations.

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I. INTRODUCTION

Let us examine the flow produced by the detonation of an unconfined right circular cylinder of high explosive, where the initiation is at a point on the central axis at one end-face (refer to Fig. 1). As the detonation progresses from the point of initiation, the gaseous explosion products expand out through the end-face. Consequently, a rarefaction wave travels into the gas behind the detonation front. When the detonation reaches the side of the cylinder, a shock is transmitted into the surrounding medium and a lateral rarefaction wave is reflected into the explosion products. Subsequently, the head of the lateral rarefaction wave impinges on the central charge axis and annihilates the rear rarefaction wave. The region bounded by the head of the lateral rarefaction and the detonation front is sometimes referred to as the "detonation head".^{1*}

While considerable attention has been given to the detonation head, there does not appear to be in the literature any attempt to calculate the actual flow in the detonation head region. With the use of the Naval Ordnance Laboratory's two-dimensional hydrodynamics computer program, CYCLONE², a detailed numerical analysis of this transient compressible flow problem can be carried out. The results of calculations for a two-inch diameter cylinder of pentolite (50/50 PETN/TNT) explosive are presented in Sec. V of this report. The calculations were performed on an IBM-7090 computer.

* References are on Page 15.

II. THE PHYSICAL MODEL

We make the physical assumptions about the detonation that (1) the chemical reaction zone is infinitely thin (i. e., the solid explosive is instantaneously converted to gaseous products as the shock-detonation front passes over it), (2) the Chapman-Jouquet (CJ) conditions³ hold at the detonation front, (3) the detonation propagates in all directions from the point of initiation with the CJ detonation velocity,* (4) the explosive is surrounded by a vacuum, and (5) "edge" effects are negligible. Here, the term "edge" effects refers to the radical change in the curvature of the detonation front near the cylindrical surface of the charge. This effect is produced by the influence of the lateral rarefaction wave on the chemical reaction zone.

In solid high explosives, the width of the chemical reaction zone is of the order of several millimeters and therefore assumption (1) does not impose a too unreal restriction on the physical model. Assumption (1) does, however, eliminate any effect of the lateral rarefaction wave on the chemical reaction zone at the sides of the cylinder. Hence, assumption (5) results as a natural consequence of (1). In the experiments by Cook, et al.¹, the edge effect did not exceed 2 mm in any case. Assumption (2) is introduced into the calculations via the equation of state of the detonation-product gas (see Sec. IV).

* The CJ detonation velocity is defined as $D = V_1 [(p_2 - p_1)/(V_1 - V_2)]^{\frac{1}{2}}$, where p_1, V_1 (p = pressure, V = specific volume) is the initial state of the solid unreacted explosive and p_2, V_2 is the point of tangency of the Rayleigh line from p_1, V_1 to the reactive Hugoniot of the product gas. This is the theoretical maximum steady-state velocity which the detonation can achieve. See Ref. (3).

The shape of the detonation front directly affects the flow in the region behind the wave front. Assumption (3) imposes the requirement that the wave front coincide with the surface of an expanding sphere, whose radius of curvature is equal to the product of the CJ detonation velocity (D_{CJ}) and the time (t) elapsed after initiation. Cook, et al.,¹ and Jaffe and Clairmont⁴, show experimentally that in point-initiated cylinders of "ideal" explosives* the detonation front is indeed initially spherical, and that the radius of curvature of the front is $D_{CJ}t$. However, there is a fundamental difference between the two sets of data. In the work by Cook, et al., the radius of curvature of the detonation front approaches a constant value by the time the wave has propagated a distance of less than four charge diameters from the point of initiation. From this point on, the detonation front propagates in a "steady state" condition. In the experimental work by Jaffe and Clairmont with two-inch diameter tetryl cylinders, the radius of curvature of the detonation front increases geometrically (radius = $D_{CJ}t$) at a distance of four charge diameters from the point of initiation with no indication of reaching a steady state. In the computer calculations which are described in this report, the mathematical model of the detonation is consistent with both sets of data, since the calculations were only carried out until the detonation front is at 1.71 charge diameters from the point of initiation. There is, however, an obvious extrapolation of the calculations which can be made in the light of the Jaffe-Clairmont experimental results. This is done in Sec. VI.

* We define an "ideal" explosive as one in which the detonation propagates at the theoretical maximum steady-state velocity (i.e., the CJ detonation velocity).

III. THE HYDRODYNAMIC EQUATIONS AND THE MATHEMATICAL MODEL

We can write the hydrodynamic equations for transient, isentropic, axially symmetric flow in Lagrangian form as follows: Denote the Lagrangian coordinates by k, l , the Eulerian coordinates by R, Z , the velocity components by u, v , the density by ρ , the specific volume by $V = (1/\rho)$, the internal energy by E , the pressure by p , and the time by t . Then the equations are

$$\text{(continuity)} \quad \frac{\rho_0}{\rho} = \frac{R A}{R_0 A_0}, \quad (1)$$

$$\text{where} \quad A = \frac{\partial(R, Z)}{\partial(k, l)}, \quad (2)$$

$$\text{(momentum)} \quad \frac{d^2 R}{dt^2} = \frac{-R}{\rho_0 R_0 A_0} \left[\frac{\partial p}{\partial k} \frac{\partial Z}{\partial l} - \frac{\partial p}{\partial l} \frac{\partial Z}{\partial k} \right], \quad (3)$$

$$\frac{d^2 Z}{dt^2} = \frac{-R}{\rho_0 R_0 A_0} \left[\frac{\partial p}{\partial l} \frac{\partial R}{\partial k} - \frac{\partial p}{\partial k} \frac{\partial R}{\partial l} \right], \quad (4)$$

$$u = \frac{dR}{dt} = \int \frac{d^2 R}{dt^2} dt, \quad v = \frac{dZ}{dt} = \int \frac{d^2 Z}{dt^2} dt,$$

$$R = \int \frac{dR}{dt} dt, \quad Z = \int \frac{dZ}{dt} dt,$$

$$\text{(energy)} \quad \frac{\partial E}{\partial t} = -p \frac{\partial V}{\partial t} \quad (5)$$

where the subscript zero refers to the initial state of the material.

The equation of state for each material is assumed given in the form

$$p = p(E, V).$$

The von Neumann-Richtmyer finite difference method,¹ which handles shocks automatically, is used for the numerical integration of the hydrodynamic equations. In this scheme, an artificial

dissipative term is introduced into the conservation of energy and momentum equations. This term causes shocks to have a finite thickness and makes the flow variables change abruptly but continuously through the region of the shock. In addition, the correct entropy change is effected across the shock. In CYCLONE, the artificial dissipative term is defined as

$$q = \frac{b A}{V V_0^2} \left(\frac{\partial V}{\partial t} \right)^2 \quad (6)$$

where the variables A , V , and t are defined above and b is the shock-width constant, which can be adjusted to give the desired sharpness to the shock. The pressure, p , in equations (3), (4), and (5) is then replaced by $P = (p+q)$. The finite difference analogues of the hydrodynamic equations which are actually used in the numerical integration, can be found in Ref. 2.

Let us now briefly examine the mathematical model that is used in the finite difference method. As a result of the cylindrical symmetry, the three-dimensional flow can be represented by the flow in any R, Z ($R \geq 0$, $\theta = \text{const}$) half plane (Fig. 2). Lagrangian coordinate (k, l) lines, imbedded in the material, divide the material into zones. Initially, the mass of each zone is calculated. This mass remains constant throughout the computations, thus assuring conservation of mass. There is then assigned to each mesh point (intersection of a k and an l line) a mass equal to one-fourth of the mass in the four surrounding zones. The velocity components of each

mass point and the pressure, internal energy, and density of each zone are given as initial conditions.

At each computation cycle, the program calculates consecutively for each zone ρ from the continuity equation, E and p from the simultaneous solution of the energy equation and the equation of state, and q from the formula given in eq. (6). At this point, a time step for the integration is determined from stability conditions.⁶ The accelerations of each of the mass points are next determined by the momentum equations. From the accelerations and the time step, the new velocity components and positions of the mass points are then obtained. The calculations are advanced in finite increments of time by repeating the above steps at every integration cycle. The material flow is thus determined by the motion of the mass points.

A programmed detonation scheme is used to instantaneously convert the solid high explosive to gaseous explosion products. Since we assume the detonation propagates with the constant CJ velocity from the point of initiation, we therefore can calculate the position of the detonation surface at each computation cycle. For each zone containing solid explosive, a test is made to see if the detonation front has arrived at the zone (corner nearest the point of initiation). If it has arrived, the chemical energy of the solid explosive which is contained in the zone is added to the internal energy of that zone*. For this and subsequent time cycles, this zone uses the equation of state for the gaseous explosion products. If the detonation has not

* In the reported calculations (Sec. V), the chemical energy was actually added in discrete amounts of $1/3$ the total chemical energy in the zone as the detonation front passed over each $1/3$ section of the diagonal of the zone. By allowing the energy adjustment to take place over several computation cycles, the typical oscillations found in numerical calculations of this type were greatly reduced.

yet arrived, the equation of state of the solid unreacted explosive is used.

IV. EQUATIONS OF STATE

In compressible fluid flow calculations, it is necessary to have an equation of state for each material. The equations of state which are used for the solid unreacted explosive and the detonation product gases are discussed in this section.

When making numerical hydrodynamic calculations, it is often a satisfactory approximation, at least for solids, to use the shock Hugoniot (the locus of possible states which are attainable from some initial state by a single shock transition) as an equation of state. The equation of state for the solid unreacted Pentolite explosive is taken as

$$p = 0.1282 \mu + 1.193 \mu^3, \quad (7)$$

where p is the pressure (megabars), $\mu = \rho/\rho_0 - 1$, and ρ is the density (g/cm^3). The subscript zero refers to the initial state. Equation (7) may not closely represent the shock Hugoniot for unreacted pentolite. It is probably more representative of the shock Hugoniot for unreacted Composition B explosive (see, for example, Ref. (7)). However, almost any reasonable form for the equation of state is adequate for our calculations since the detonation is programmed as a function of time and does not depend on the state of the solid explosive. The form of the equation of state for the solid explosive has essentially no effect on the flow in the detonation-product gases.

The equation of state of the pentolite detonation-product gas is assumed to be given in the form⁸

$$p = (A\rho + B\rho^2) E + C\rho^3 \quad (8)$$

where A, B, and C are constants and p, E, and ρ are the thermodynamic variables described above. The value $A = 0.35$ is obtained by defining $A = (\gamma - 1)$, where γ is the average ideal gas specific heat ratios (c_p/c_v) of the detonation products. Equation (8) thus approaches the polytropic gas equation for small ρ . The constants $B = 0.1243$ and $C = 0.01279$ were chosen so that eq. (8) would reproduce the particular CJ detonation conditions and the CJ isentrope obtained by thermochemical calculations.*

The CJ detonation conditions for pentolite ($\rho_0 = 1.65$) gotten with the thermochemical calculations are pressure $p_{CJ} = 0.2452$ megabars, density $\rho_{CJ} = 2.210$ g/cm³, sound speed $c_{CJ} = 0.5714$ cm/ μ sec, and detonation velocity $D = 0.7655$ cm/ μ sec. The value of the CJ specific internal energy $E_{CJ} = 0.0775$ megabar-cm³/g is obtained by calculating the area under the CJ isentrope from the CJ pressure to zero pressure. The chemical energy E_0 which is used in the computer calculations is obtained from the Hugoniot relation

$$E_{CJ} - E_0 = (p_{CJ} + p_0) (V_0 - V_{CJ})/2. \quad (9)$$

This gives $E_0 = 0.0587$ megabar-cm³/g. E_0 is the energy which is added to the specific internal energy of a zone as the detonation front reaches the zone (see Sec. III).

* The thermochemical calculations were carried out by H. Hurwitz, using the RUBY computer program⁹ which contains the Cowan-Fickett version of the Becker-Kistiakowsky-Wilson equation of state¹⁰. The modified RDX parameters of Mader¹¹ were used in the calculations.

V. RESULTS OF CALCULATIONS

The results of the calculations on the flow produced by the detonation of a two-inch cylinder of pentolite explosive are summarized in Figs. 3-12. Figures 3-10 and 12 were processed directly from the computer calculations (excluding the labels and dashed-in rarefaction fronts) on a Stromberg-Carlson SC-4020 Microfilm Recorder.

The cross section (parallel to the central axis) of the detonating cylinder is shown in Figs. 3-6 for different instants of time after initiation. Initiation of the detonation is at $t=0$. The Lagrangian computation grid is plotted on the cross section. The initial grid (Fig. 3) consists of approximately 4000 mesh points. Additional grid is generated as the detonation progresses down the cylinder. At $t = 11.3841$ microseconds the computation grid has 9000 mesh points (the top half of the grid shown in Fig. 6). The initial zone size of the solid explosive is 0.0508×0.05 cm. Individual zones in the solid explosive and the compressed explosion products cannot be clearly distinguished in the figures because of the inadequate resolution of the scale which was chosen for the plots. In Figs. 4-6, however, the zone configuration is discernible in the region where the gas has undergone some expansion. At 2.9753 microseconds after initiation (Fig. 4), the detonation has not yet reached the side of the cylinder. The detonation-product gas expands only out the end-face of the cylinder. After the detonation reaches the side of the cylinder (Fig. 5) the gas expands radially as well. The cross section at $t = 11.3841$ microseconds is shown in Fig. 6. The

Lagrangian grid line which was originally the end-face surface of the solid explosive was dropped from the calculations at $t = 9.9171$ microseconds and therefore does not appear in Fig. 6.

The pressure distribution in the product gas at specific times after initiation is illustrated in Figs. 7-10. Here, the positions of the isobars in the cross section of the detonation are shown. The leftmost isobar is the 10 kilobar line. On each consecutive isobar to the right, the pressure increases by 10 kilobars. The detonation front is at the CJ pressure of 245 kilobars. The head of the rear and lateral rarefaction waves are shown by dashed lines. The head of the lateral rarefaction wave can be located on each isobar (≥ 60 kb) at the point where the isobar departs from being circular. On the central axis, the head of the rear rarefaction wave moves with the 55 kb isobar. In Fig. 7, only the rear rarefaction wave exists. In Figs. 8 and 9, both rarefactions can be seen. The head of the lateral rarefaction impinges on the central axis at $t = 11.3841$ microseconds (Fig. 10), thereby annihilating the rear rarefaction wave. At subsequent times, the head of the rear rarefaction wave does not appear.

It should be noticed that the flow is entirely spherical in the region (detonation head) bounded by the heads of the rear and lateral rarefaction waves and the detonation surface. Moreover, this spherical flow is exactly that which is described by the similarity solution of G. I. Taylor for a spherical detonation¹² (Hereafter referred to as the spherical Taylor wave). In Fig. 11, the pressure and particle velocity profiles along the central axis in the CYCLONE

calculations ($t = 7.6359$ microseconds) are compared to the pressure and particle velocity distribution in a spherical Taylor wave.* The two sets of data are shown to be in exact agreement in the region where the Taylor wave particle velocity is greater than zero. The departure of the two data in the Taylor wave region of zero particle velocity is due to the two different boundary conditions at the initiation point. In the Taylor similarity solution the detonation is spherical and the geometry imposes the boundary condition that the gas at the point of initiation remain fixed. In the CYCLONE calculations the detonation is hemispherical and the gas at the point of initiation on the central axis is allowed to expand freely.

The expansion of the gas along the axis causes a rarefaction wave to follow the detonation front. This rear rarefaction wave exists only until it is annihilated by the lateral rarefaction wave impinging on the central axis. Previous to this time, the penetration of the rear rarefaction wave, along the axis, is known since the position of the head of this wave must correspond with the "sonic point" (point of zero particle velocity) in the Taylor wave. We see from Fig. 11 that this is so.

* This Taylor wave was numerically generated with the use of W. A. Walker's computer routines¹³. The equation of state for the detonation products given in Sec. IV was used in the Taylor wave calculations.

The effect of the von Neumann-Richtmyer finite difference method on the flow variables at the shock front is demonstrated in Fig. 11. The pressure and particle velocity profiles are "rounded" at the shock front and a small "tail" precedes the actual position of the shock front. This typical characteristic of the numerical method produces an inherent "edge" effect in the calculations. The "tail" causes the unreacted explosive at the cylindrical surface to expand before it is "detonated" by the computer program. Therefore the lateral rarefaction wave proceeds into the cylinder about 0.3 microseconds sooner than it would if the shock-detonation front were infinitely thin.

The specific volume (or density, since $\rho = 1/V$) distribution in the cross section of the detonating cylinder at $t=11.3841$ microseconds is shown in Fig. 12. The isochore furthest from the detonation front is $V=1.50 \text{ cm}^3/\text{g}$. The specific volume decreases by $0.05 \text{ cm}^3/\text{g}$ on each consecutive isochore closer to the detonation front. At the detonation front, the specific volume is $V=1/\rho_{\text{CJ}}=1/2.210=0.4525 \text{ cm}^3/\text{g}$. The specific volume distribution in the detonation head region is identical to the specific volume distribution in a spherical Taylor wave.

VI. DISCUSSION

The results of the calculations (Sec. V) are, of course, only valid for that part of the detonation where our physical and mathematical model of the detonation is consistent with the experimental data. More specifically, it is valid over that region where the shape of the detonation front can be represented by an expanding sphere of radius $D_{\text{CJ}}t$. From the extensive experimental data of Cook,

et al¹., this is shown to be for a charge length of 3.5 charge diameters for pentolite, in particular, and for charge lengths of 1 to 4 charge diameters for solid explosives, in general. Since the calculations were carried out to where the detonation front was 1.71 charge diameters from the point of initiation, we are well within the limitations of our model.

In addition to the specific numerical results obtained, more general conclusions can be made. We have shown that the flow immediately behind the detonation front in the region unaffected by the rear and lateral rarefaction wave, is, identically, the Taylor similarity flow for a spherical detonation. Since the characteristic of similarity flows is that the flow variables depend only on their relative position in the flow, we are able to determine the flow in this region for later times. That is, at least to the point where the radius of curvature of the detonation front is equal to 3.5 charge diameters which is the upper limit of our detonation model according to Cook's data. From the rather limited experimental data of Jaffe and Clairmont⁴, the indication is that our model of the detonation may hold over a much greater distance. Therefore, perhaps, the Taylor similarity solution may be validly extended to charge lengths greater than 3.5 charge diameters.

It should be pointed out that although one can obtain the flow in the detonation head region for later times because it is a similarity flow, one cannot, however, determine the shape of this region by extrapolating the calculated results. The shape of the detonation head has to be determined by calculating the motion of the lateral rarefaction front into the spherical Taylor wave flow of the detonation head.

VII. ACKNOWLEDGEMENTS

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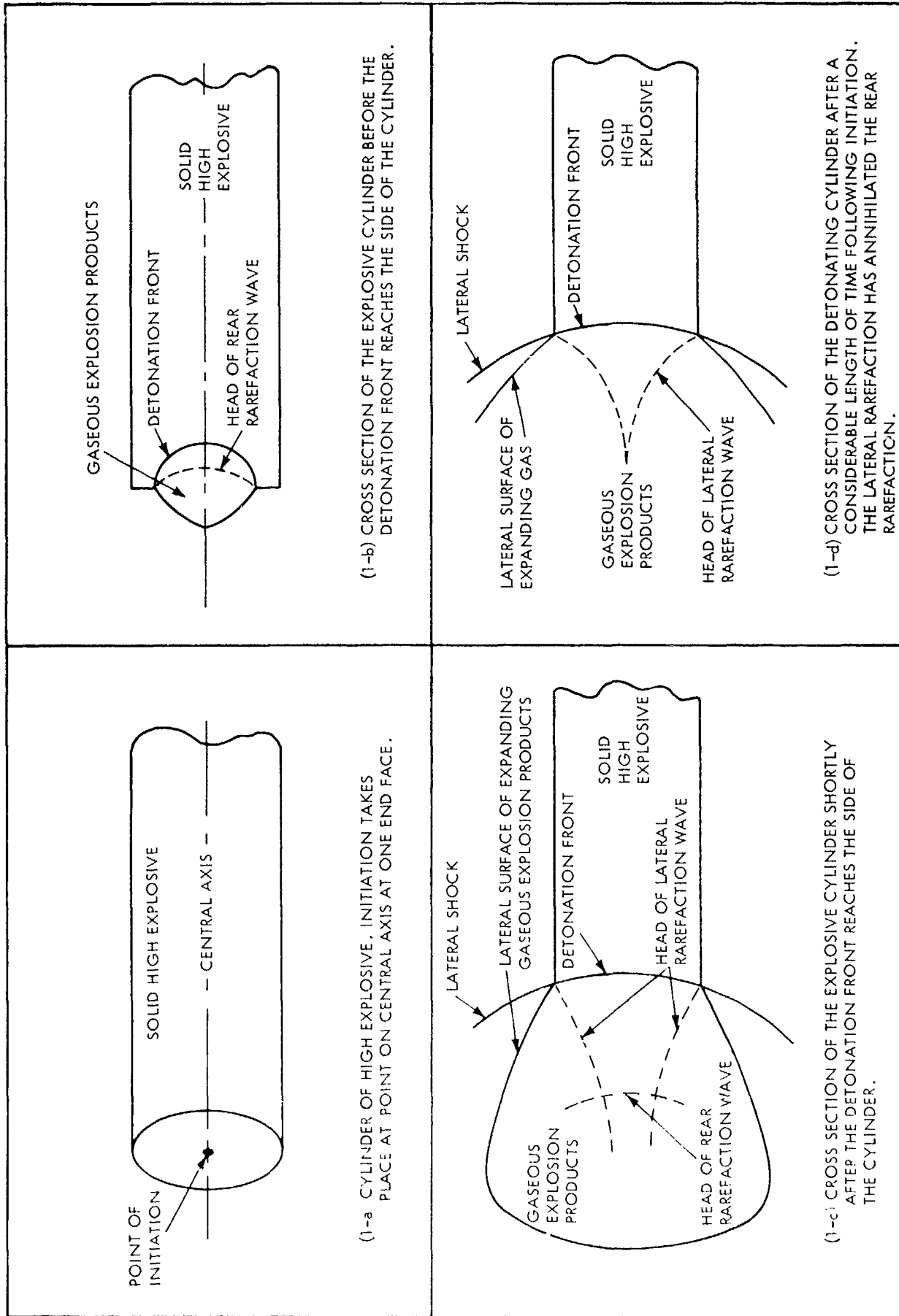


FIG. 1 A QUALITATIVE DESCRIPTION OF THE FLOW IN A POINT-INITIATED CYLINDER OF EXPLOSIVE

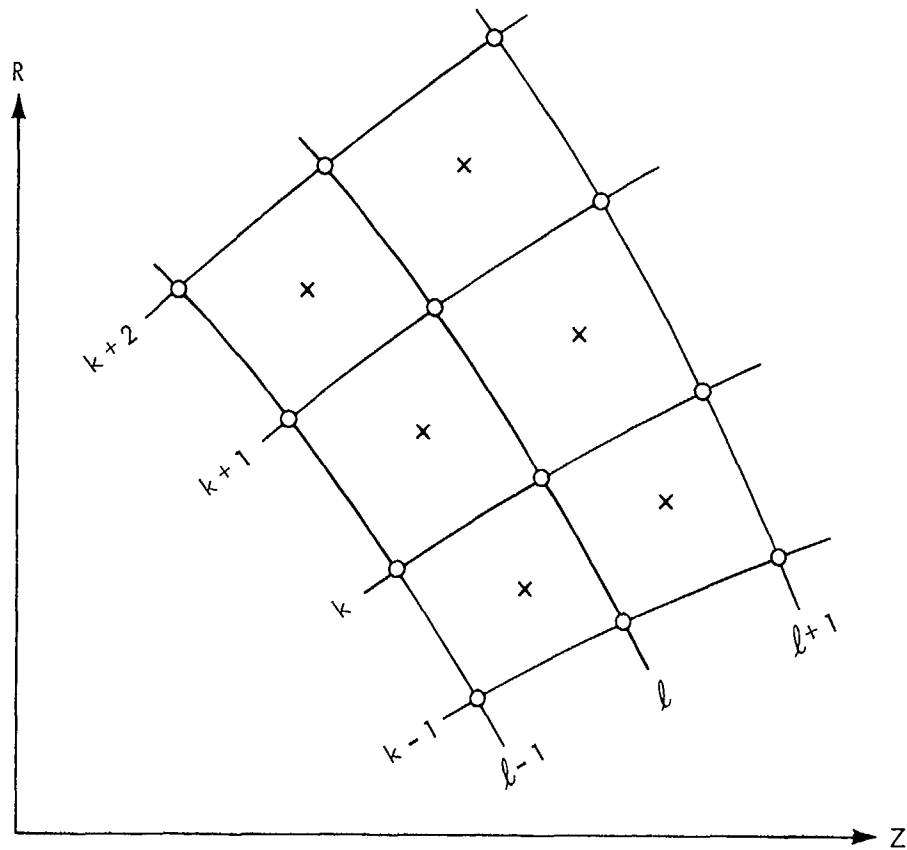


FIG. 2 A GENERAL LAGRANGIAN COMPUTATION GRID. MASS POINTS ARE LOCATED AT THE INTERSECTION OF THE k, l LINES. POSITIONS AND VELOCITIES ARE ASSOCIATED WITH EACH MASS POINT. PRESSURE, SPECIFIC VOLUME, INTERNAL ENERGY, AND AN ARTIFICIAL VISCOSITY ARE LOCATED AT THE CENTER (X's) OF THE QUADRILATERALS ("ZONES").

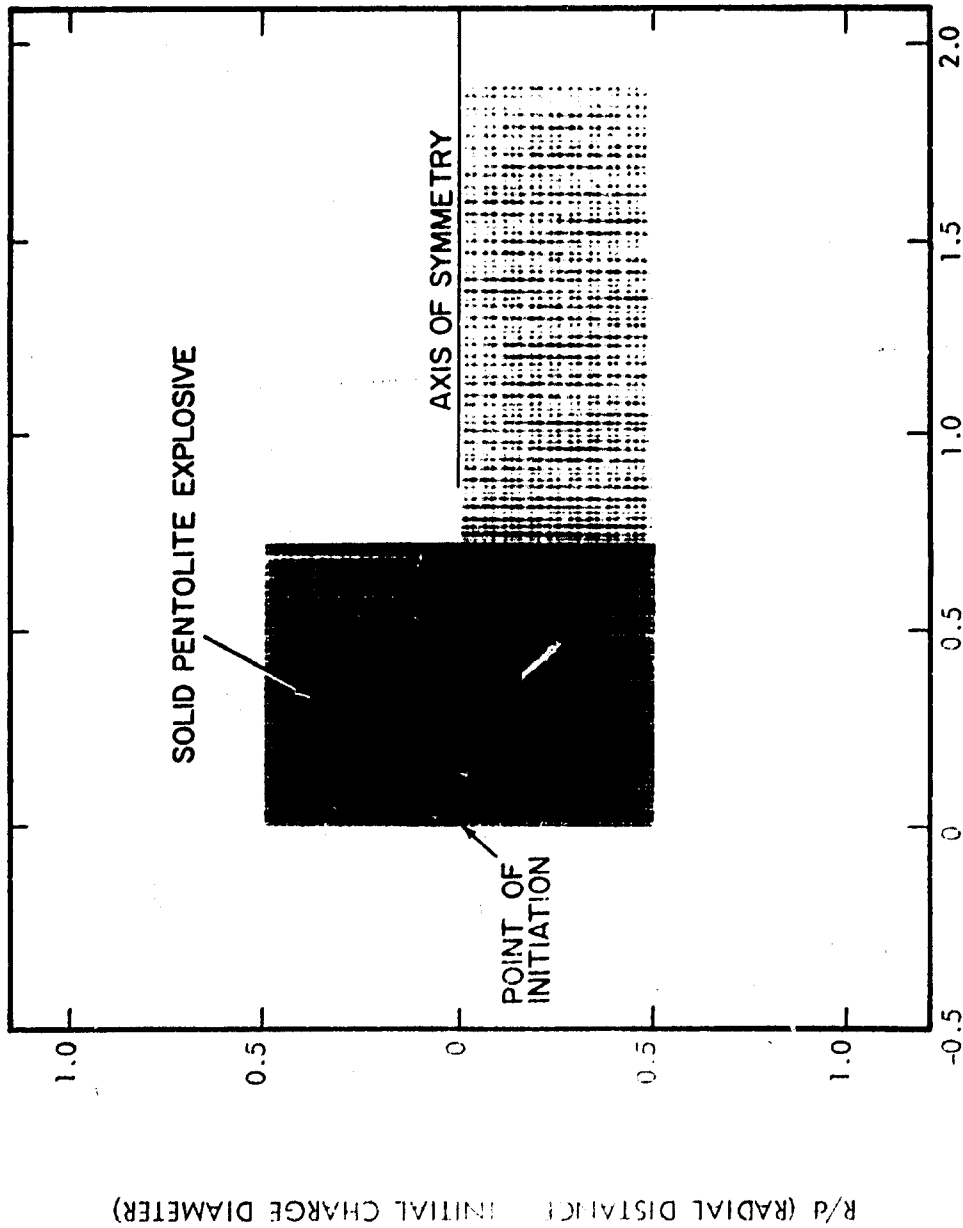


FIG. 3 Cross section of a two inch diameter cylinder of pentolite.

The initial Lagrangian computation grid is shown on the cross section. The computations are made with the half of the grid which is above the axis of symmetry. The bottom half of the grid is plotted as the mirror image of the top half. The point of initiation is at $(R/d, Z/d) = (0, 0)$.

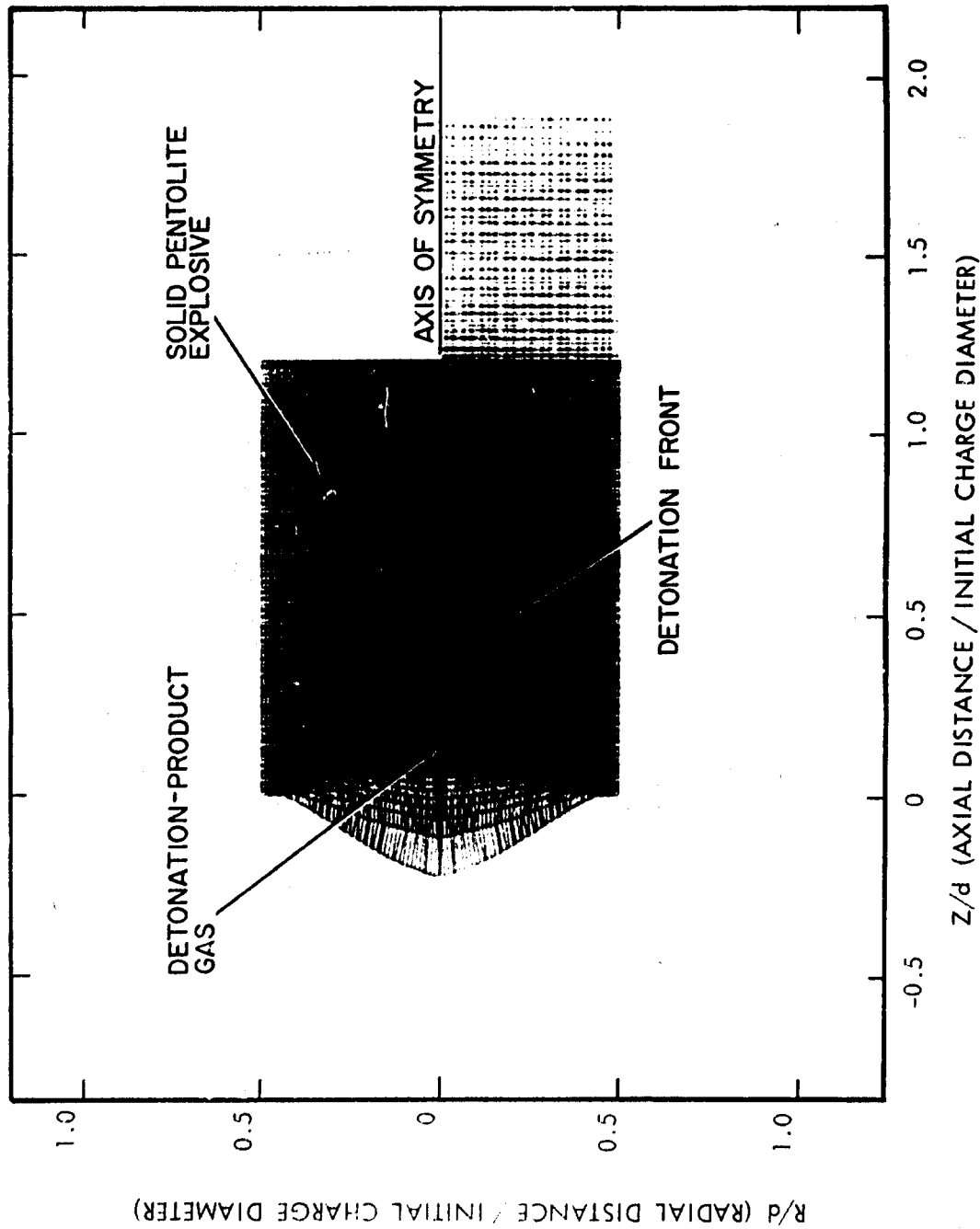


FIG. 4 Cross section of the detonating cylinder at 2.9753 μ seconds after initiation. The detonation front has not yet reached the side of the cylinder. Point of initiation is at $(R/d, Z/d) = (0,0)$.

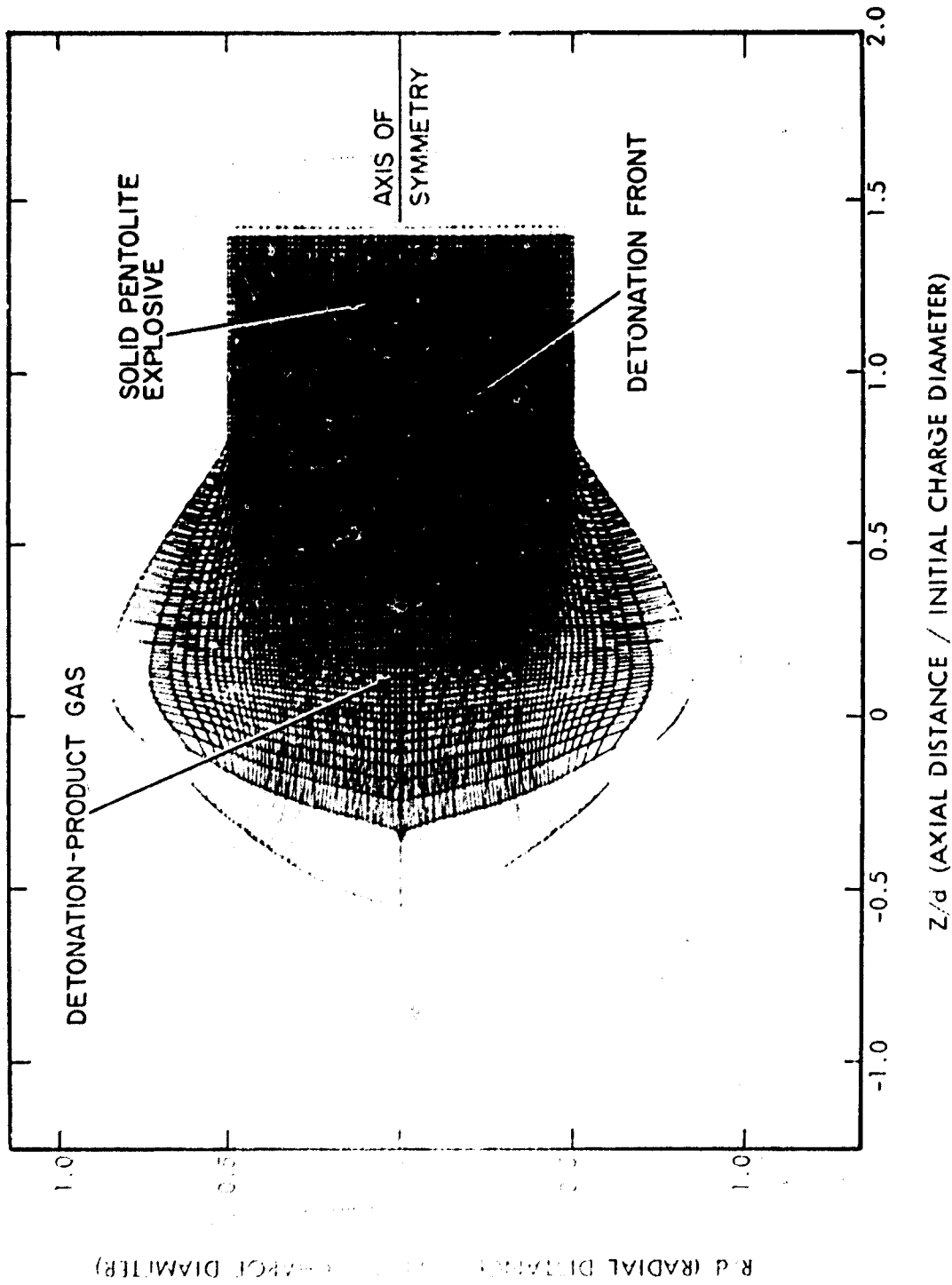


FIG. 5 Cross section of the detonating cylinder at 6.249 μ seconds after initiation. The detonation front has reached the side of the cylinder and the detonation-product gas expands radially. Point of initiation is at $(R/d, Z/d) = (0, 0)$.

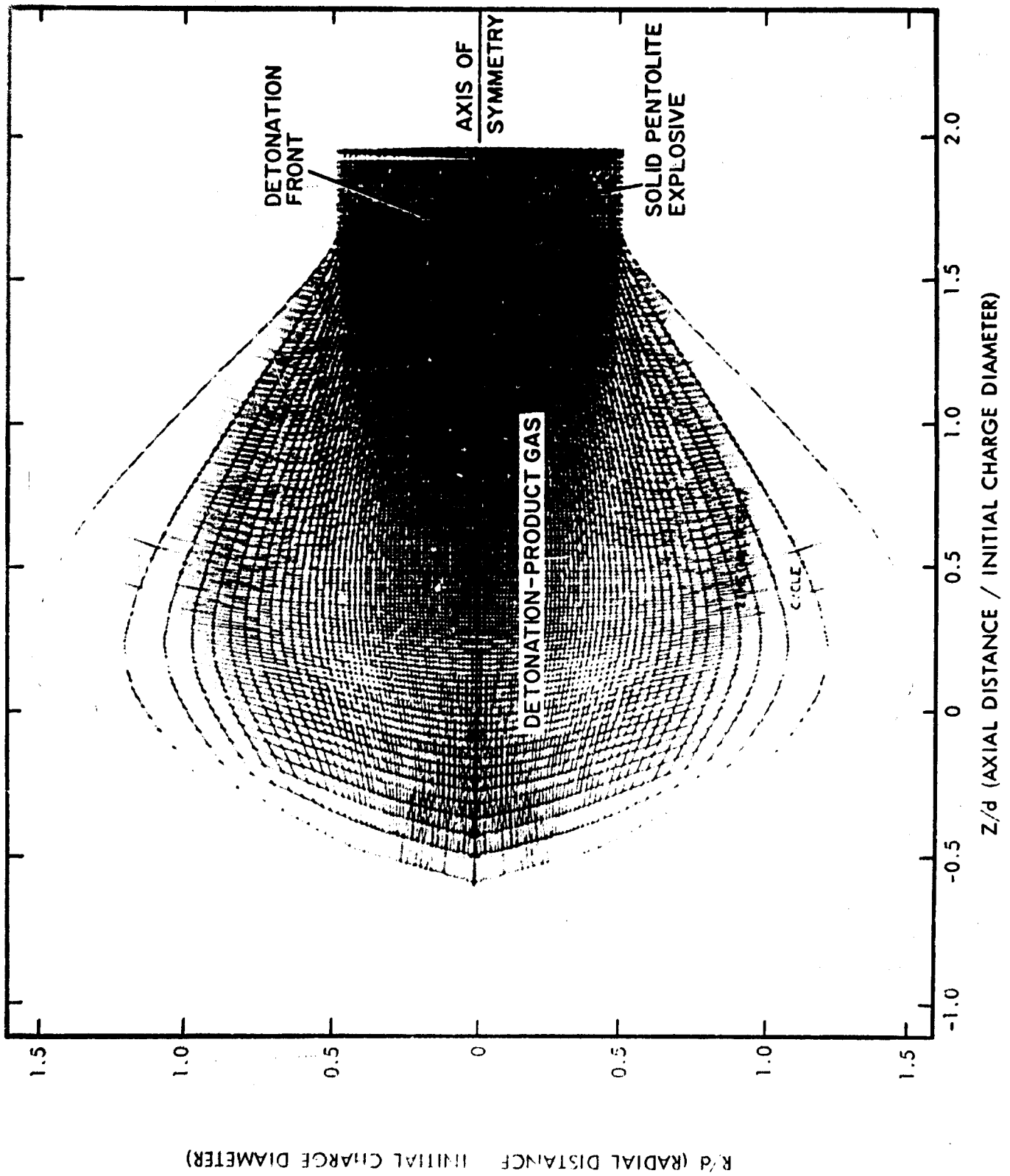


FIG. 6 Cross section of the detonating cylinder at 11.3841μ seconds after initiation. Point of initiation is at $(R/d, Z/d) = (0,0)$.

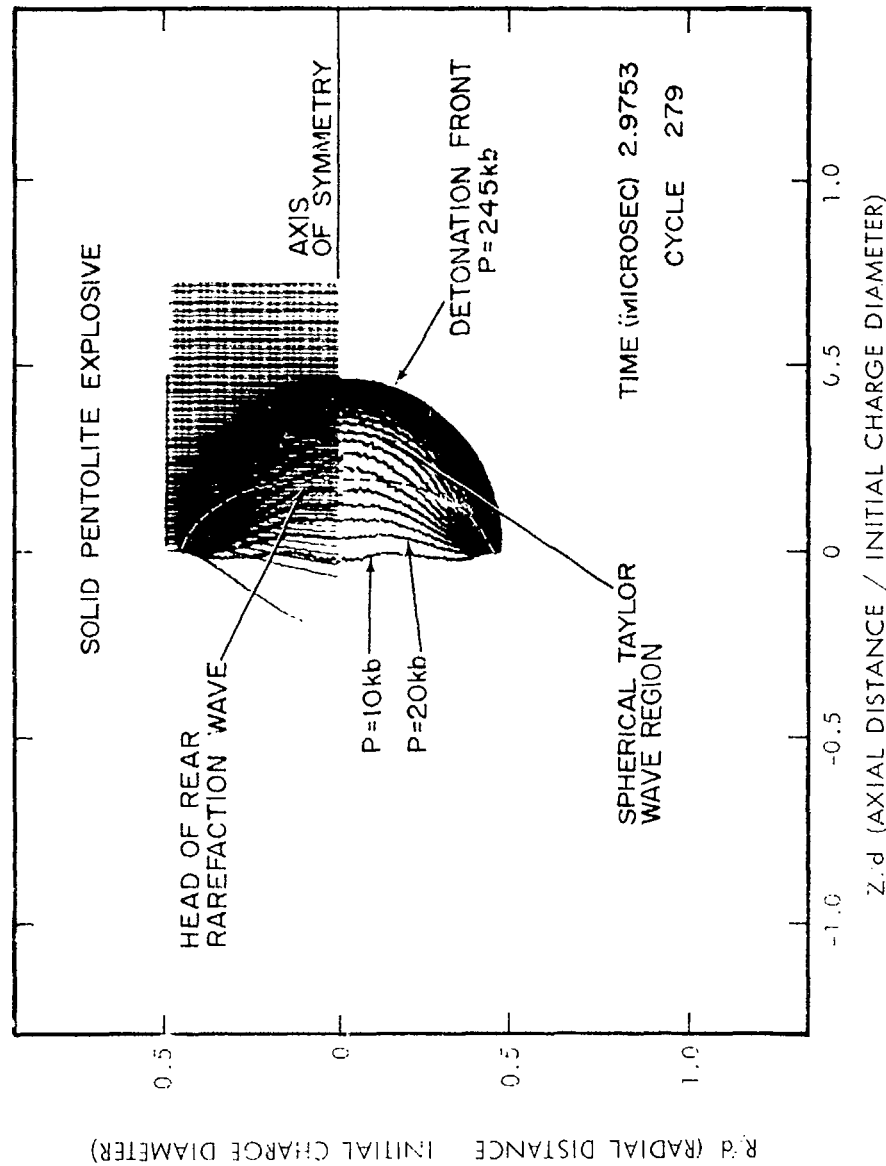


FIG. 7 The pressure distribution in the form of isobars is shown in the cross section of the detonating cylinder at 2.9753 μ seconds after initiation. There is a difference of 10 kilobars between adjacent isobar lines (actually a set of discrete points) with the leftmost isobar = 10kb and the pressure at the detonation front = 245kb. Point of initiation is at $(R/d, Z/d) = 0, 0$.

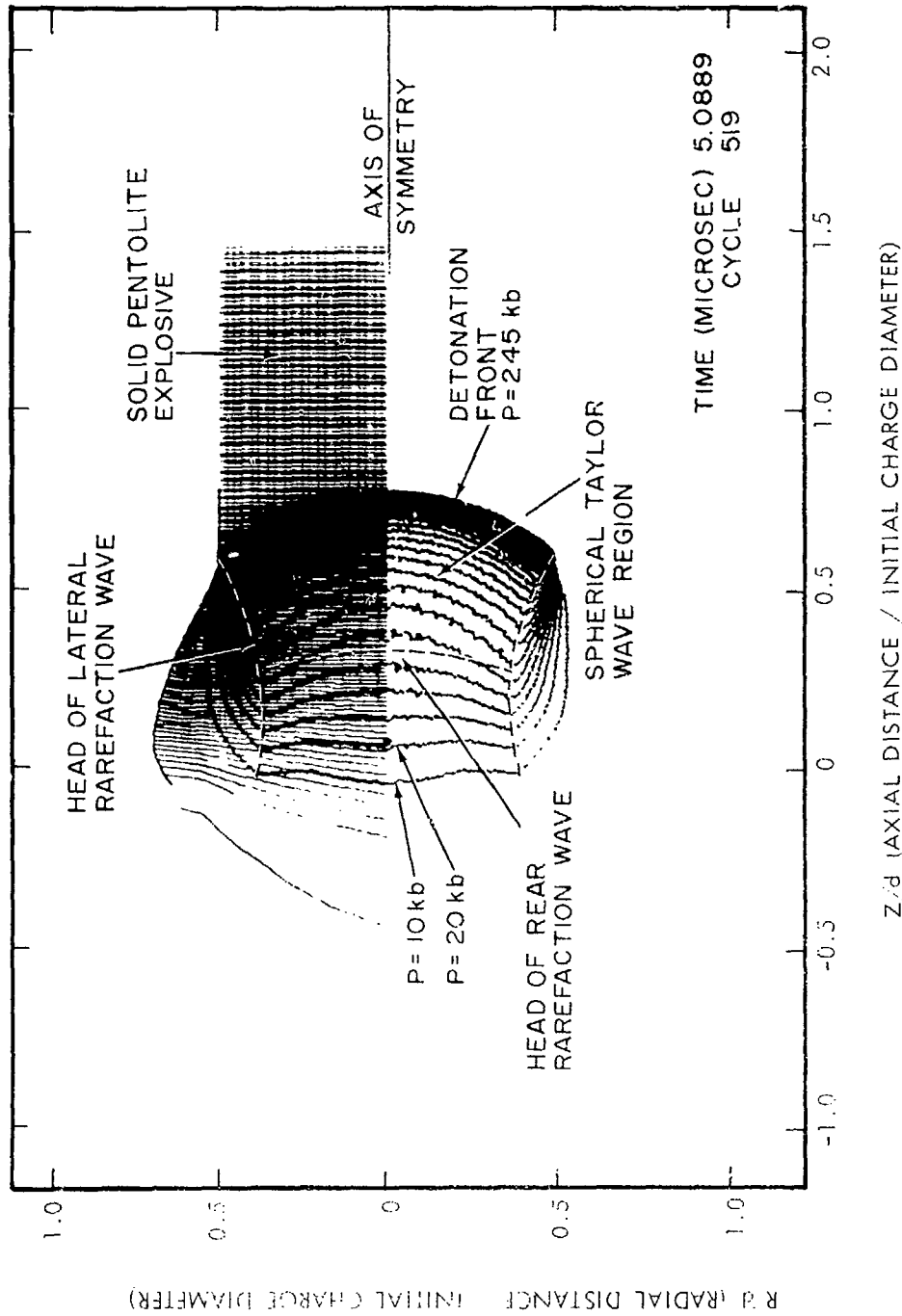


FIG. 8 The pressure distribution in the form of isobars is shown in the cross section of the detonating cylinder at 5.0889 μ seconds after initiation. There is a difference of 10kb between adjacent isobar lines. Point of initiation is at $(R/d, Z/d) = (0, 0)$.

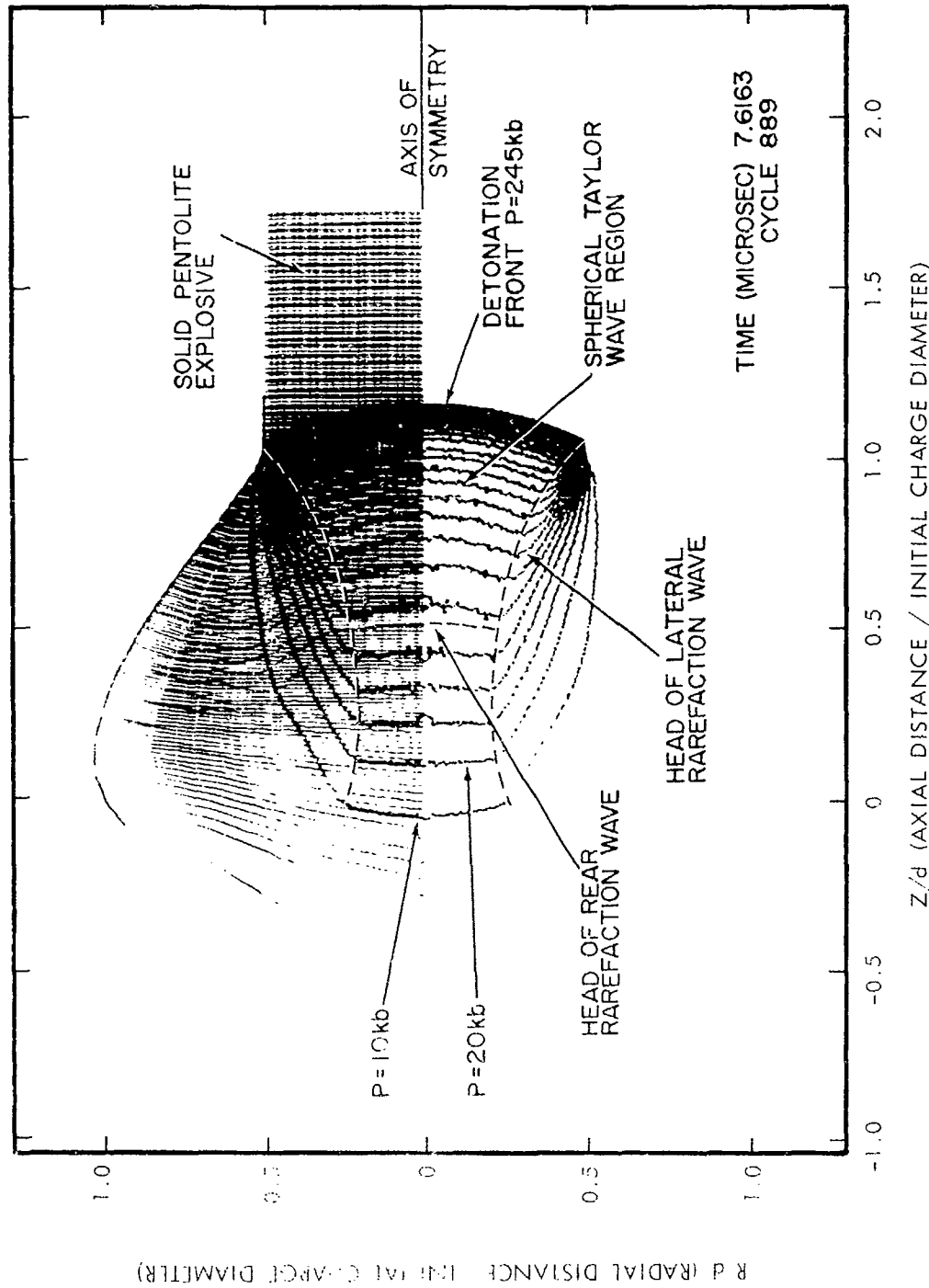


FIG. 9 The pressure distribution in the form of isobars is shown in the cross section of the detonating cylinder at 7.6163 μ seconds after initiation. There is a difference of 10kb between adjacent isobar lines. Point of initiation is at $(R/d, Z/d) = (0, 0)$.

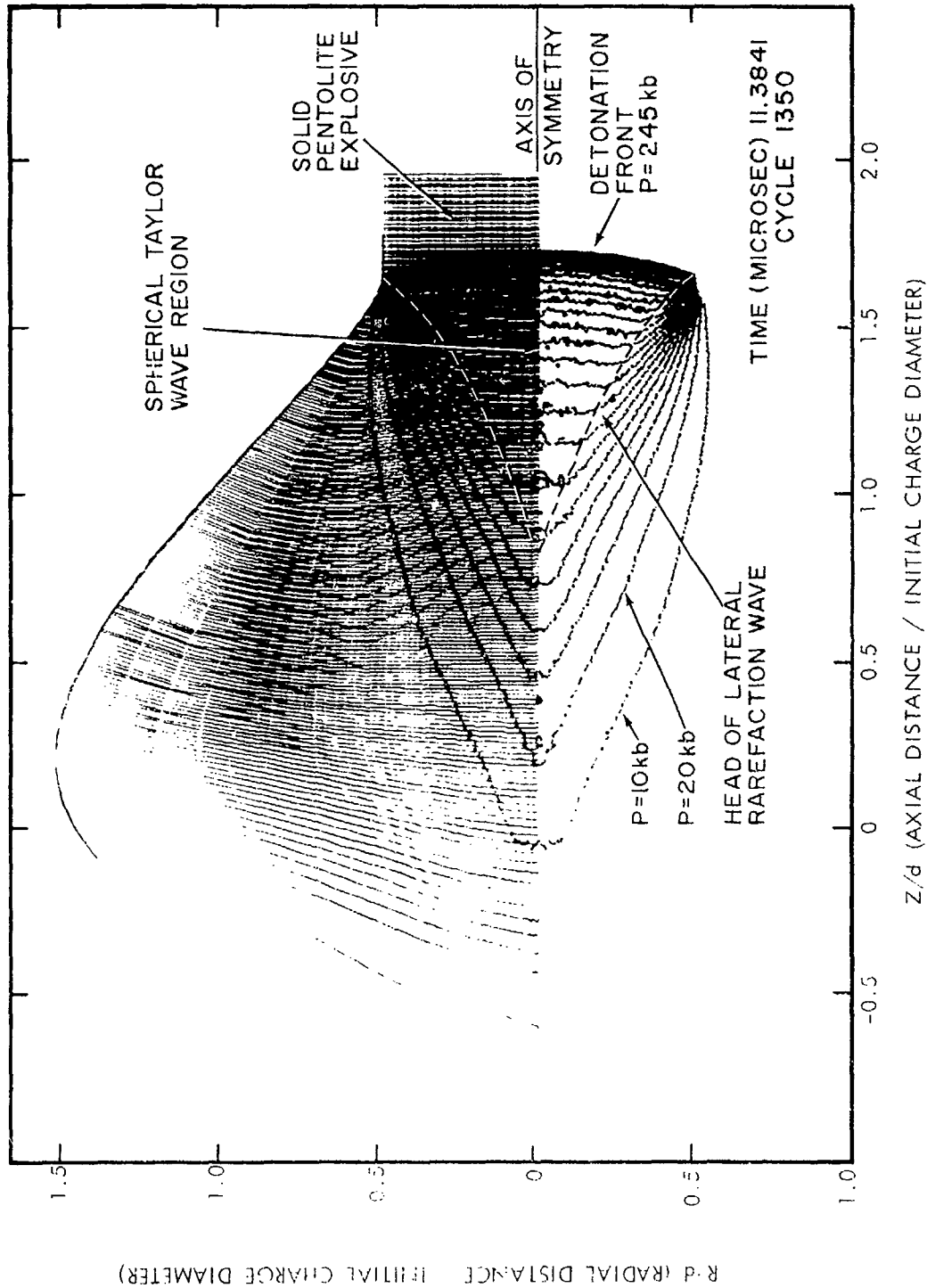


FIG. 10 The pressure distribution in the form of isobars is shown in the cross section of the detonating cylinder at 11.3841 μ seconds after initiation. There is a difference of 10kb between adjacent isobar lines. Point of initiation is at $(R/d, Z/d) = (0, 0)$.

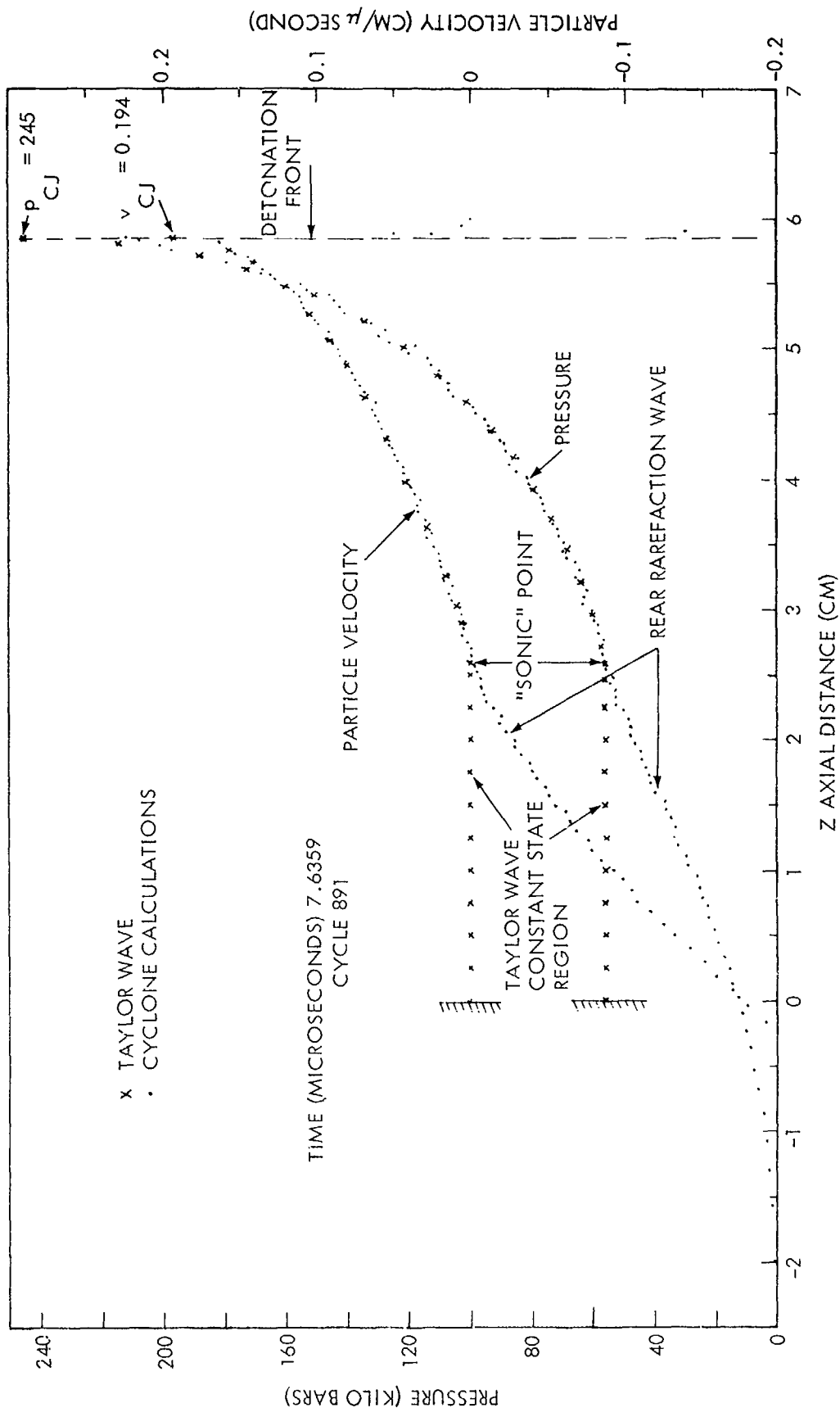


FIG. 11 Comparison of the pressure and particle velocity along the central axis (CYCLONE calculations) and the radial pressure and particle velocity distribution in a spherical Taylor wave. The CYCLONE values are taken at $t=7.6359$ microseconds after initiation. The Taylor wave was generated with the computer routines which are described in reference (13). Point of initiation is at $Z=0$.

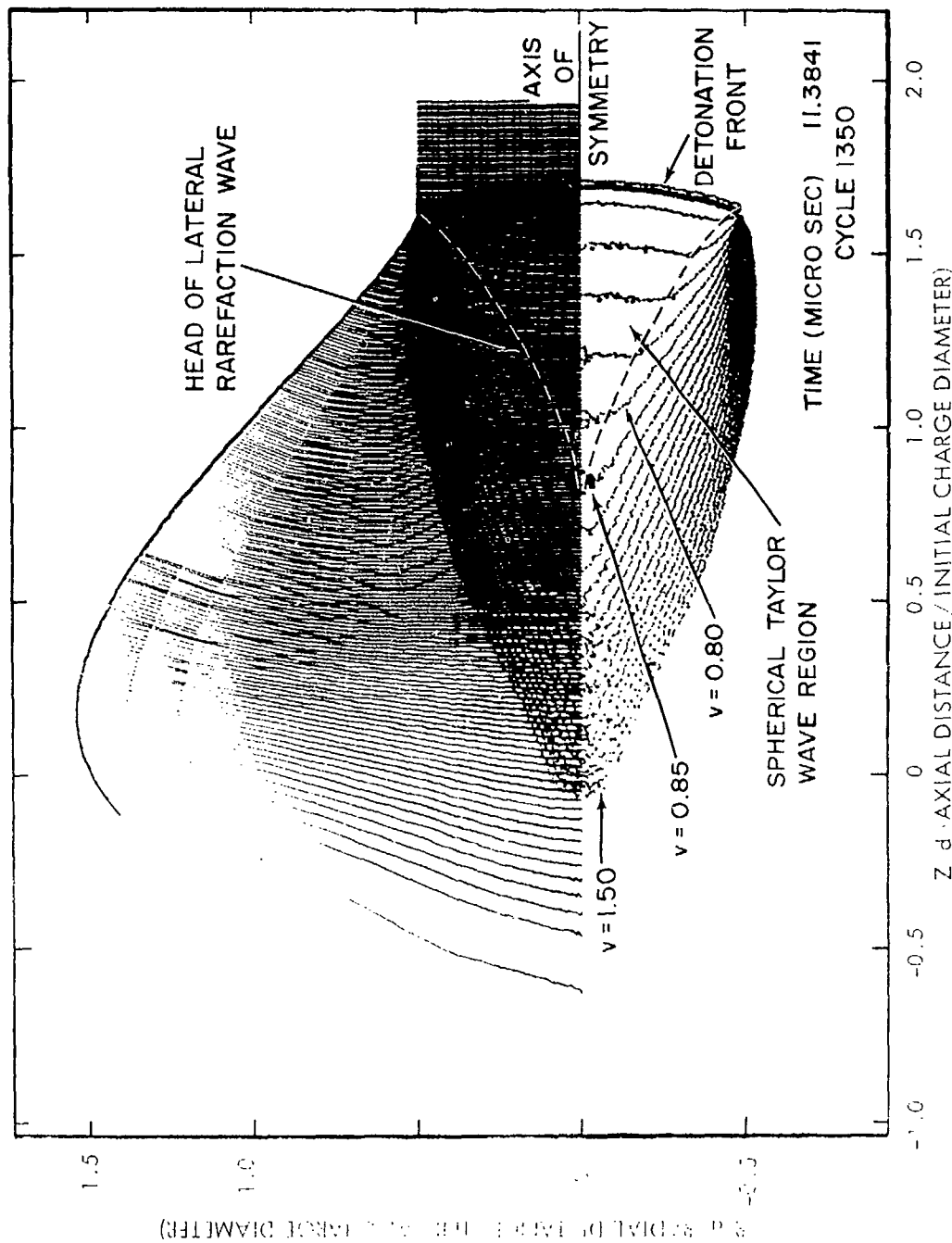


FIG. 12 The specific volume distribution in the cross section of the detonating cylinder at $t = 11.3841 \mu$ seconds. The isochore furthest from the detonation front is $V = 1.50 \text{ cm}^3/\text{g}$. The difference between isochores is $0.05 \text{ cm}^3/\text{g}$. At the detonation front, $V = 0.452 \text{ cm}^3/\text{g}$. This isochore does not appear in the figure. The three lines at the detonation front (starting from the right $V = 0.60$, 0.55 , and 0.50) are a result of the finite difference method which produces a continuous transition of the flow variables across the shock.

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